# Modeling and Simulation of Single Phase Fluid Flow and Heat Transfer in Packed Beds

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**Abstract:** Computational fluid dynamics has emerged as an advanced tool for studying detailed behavior of fluid flow and heat transfer characteristics in many of the chemical engineering applications. One such application can be found in packed beds. Packed bed systems play a very important role in most of the chemical industries, especially petroleum, petrochemical and biochemical industries. Hence it is essential to understand the fluid flow behavior and temperature variation in different sections of packed bed. Geometric complexities of packed beds have prevented detailed modeling of their hydrodynamics. With the help of modern CFD codes and the exponential growth of computer power, it is now feasible to obtain detailed flow fields and temperature profiles in packed beds of high tube-to-particle diameter ratio. By using COMSOL Multiphysics for modeling and simulation of packed bed reactors, a detailed description of the flow behavior and heat transfer aspects within the bed can be established.

**Keywords:** Computational Fluid Dynamics, Heat Transfer, Packed Bed, Spherical Packing, Single Phase, Newtonian, N factor, Incompressible, Turbulent Flow, Steady State.

## 1. Introduction

In chemical processing, a packed bed is a hollow tube, pipe, or other vessel that is filled with a packing material. The packing can be randomly filled with small objects or else it can be a specifically designed structured packing. The purpose of a packed bed is typically to improve contact between two phases in a chemical or similar process. Packed beds can be used in a chemical reactor, a distillation process, an absorption process or a scrubber, but packed beds have also been used to store heat in chemical plants.

Two major limitations of the packed bed systems are channeling and formation of hot spots. There are many channels but the fluid flows through only few channels, that is, it doesn't distribute itself properly. Also, the formation of hot spots leads to damage of the bed and packing material.

From a fluid mechanical perspective, the most important issue is that of the pressure drop required for the liquid or the gas to flow through the column at a specified flow rate.

The area of study in this section not only focuses on the pressure drop issue but also encompasses velocity field of fluids and heat transfer in packed bed systems.

Computational fluid dynamics, usually abbreviated as CFD, is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. These numerical analysis methods discretize continuous equations to obtain numerical solutions. Some of these methods are finite volume method, finite element method, finite difference method, boundary element method etc. In all of these approaches the same basic procedure is followed.

Packed bed models have usually been developed for a low tube to particle diameter ratio where temperature and flow profile gradients are mild and can be averaged. One such model has been developed for N=2 and N=4 (Michiel Nijemeisland and Anthony G. Dixon, 2004). Values for pressure drop obtained from the simulations for N=2 geometry were validated against experimental values. The turbulence models used (k-ε and RSM) showed similar results, with an average error from the experimental values of about 10%. In this study, more practical 3D models for N=4 and N=8 with structured spherical packing have been developed to get accurate results.

The study involved understanding fluid flow behavior through packed bed systems by solving related governing equations and modeling. CFD (COMSOL Multiphysics) has been used for obtaining the results which were validated with literature data.

## 2. Mathematical Modeling

### 2.1 Ergun Equation

The Ergun equation tells us a number of things. It tells us the pressure drop along the length of the packed bed given some fluid velocity. It also tells us that the pressure drop depends on the packing size, length of bed, fluid viscosity and fluid density.

$$\frac{\Delta p}{L} = \frac{150\mu(1-\beta)^2 u_o}{\beta^3 d_p^2} + \frac{1.75(1-\beta)\rho u_o^2}{\beta^3 d_p}$$

### 2.2 Equation of Continuity

The continuity equation states that the rate of increase of mass in a control volume is equal to the difference in rate of mass in and rate of mass out. The differential form of the continuity equation is:

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho \mathbf{u}) = 0$$

If $\rho$ is a constant, as in the case of incompressible flow, the mass continuity equation simplifies to a volume continuity equation:

$$\nabla.\mathbf{u} = 0$$

which means that the divergence of velocity field is zero everywhere. Physically, this is equivalent to saying that the local volume dilation rate is zero.

### 2.3 Navier Stokes Equation

The Navier Stokes equation is the equation of motion for a newtonian fluid with constant viscosity and density. The equation is greatly simplified when applied to 2D flow with the assumption that velocity is only in the axial (z) direction i.e. $v_r$=0 and $v_\theta$=0

$$-\frac{dp}{dz} + \rho g_z + \mu\left[\frac{1}{r}\frac{d}{dr}\left(r\frac{dv_z}{dr}\right)\right] = 0$$

### 2.4 Standard K-E Turbulence Model

At high Reynolds numbers the rate of dissipation of kinetic energy (ε) is equal to the viscosity multiplied by the fluctuating vorticity. An exact transport equation for the fluctuating vorticity, and thus the dissipation rate, can be derived from the Navier Stokes equation. The k-ε model consists of the turbulent kinetic energy equation.

$$\rho\left(\boldsymbol{u}.\nabla\right)k = \nabla.\left(\left[\mu + \frac{\mu_T}{\sigma_k}\right]\nabla k\right) + P_k - \rho\varepsilon$$

and the dissipation rate equation

$$\rho(\boldsymbol{u}.\nabla)\varepsilon = \nabla.\left(\left[\mu + \frac{\mu_T}{\sigma_e}\right]\nabla\varepsilon\right)$$

$$+C_{e1}P_k\frac{\varepsilon}{k} - C_{e2}\rho\frac{\varepsilon^2}{k}$$

Where $P_k$ represents,

$$P_k = \mu_T\left[\nabla\boldsymbol{u}:(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T)\right]$$

And $C_{e1}$, $C_{e2}$ and $\sigma_K$ are turbulence model parameters (constants). In the implementation of this model the Kolmogorov - Prandtl expression for the turbulent viscosity is used

$$\mu_T = \rho C_\mu \frac{k^2}{\varepsilon}$$

### 2.5 Heat Transfer (Convective)

Assuming that T varies in the axial as well as radial directions i.e T=T(r,z), the energy equation simplifies to:

$$\rho C_p\left(v_z\frac{dT}{dz}\right) = k'\left[\frac{1}{r}\frac{d}{dr}\left(r\frac{dT}{dr}\right) + \frac{d^2T}{dz^2}\right]$$

## 3. Computational Fluid Dynamics (CFD) using COMSOL Multiphysics

### 3.1 Packed Bed 3D for N=4

Packed bed with N=4 has been modeled by using COMSOL Multiphysics (4.2a). Space dimension was selected as 3D. Turbulent flow with standard k-ε model was selected in physics. Study type was chosen as stationary (steady state). A solid cylinder with diameter 10.16 cm was created. Then spheres, 2.5 cm in diameter, were drawn in accordance with N=4 with 12 spheres per layer. In this model, 9 spheres of the first layer were placed such that they touch the inner surface of the tube. The remaining 3 spheres were placed inside this arrangement such that 2 of them and 2 from the other 9 spheres lie along the diameter and the last sphere lies in between this arrangement. The second layer had the similar geometry and the two layers were placed such that they stack over each other as shown in Figure 1.

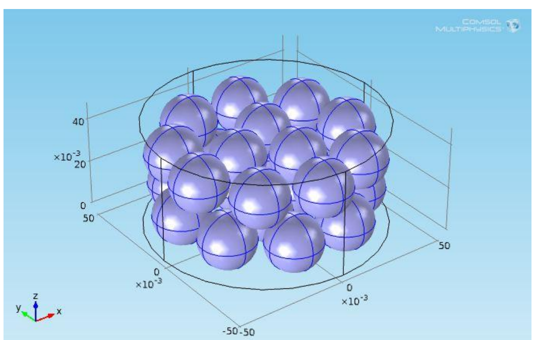

**Figure 1:** N=4 Geometry

The Sub-domain was specified as air at 293.15 K and 1 atm. The boundary conditions were then specified. One cross section served as the inlet with velocity 1.0624 m/s and temperature 300 K while the other served as the outlet with zero gauge pressure, no viscous stress and thermal insulation. The remaining surfaces were set as walls with wall function condition. The cylindrical wall was maintained at a constant temperature of 400 K and the spheres were maintained at a constant temperature of 300 K. Extra coarse meshing (85307 elements) was used and the model was simulated using COMSOL (4.2a) to obtain the results.

### 3.2 Packed Bed 3D for N=8

Packed bed with N=8 has been modeled by using COMSOL Multiphysics (4.2a). Space dimension was selected as 3D. Turbulent flow with standard k-ε model was selected in physics. Study type was chosen as stationary (steady state). A solid cylinder with diameter 10.16 cm was created. Then spheres, 1.27 cm in diameter, were drawn in accordance with N=8 with 47 spheres per layer. In this model, 20 spheres of the first layer were placed such that they touch the inner surface of the tube. 3 spheres were placed exactly in the center and the remaining 24 spheres were placed in the annular region. A similar layer was created and the two layers were placed such that they stack over each other as shown in Figure 2.

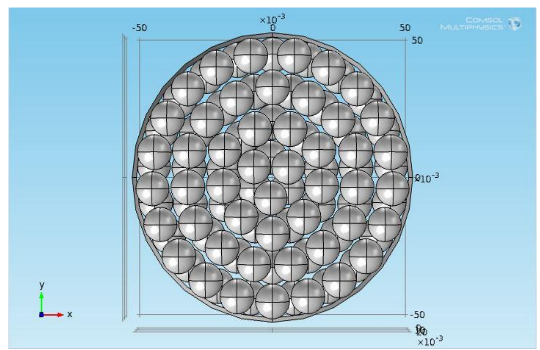

**Figure 2:** N=8 Geometry

The Sub-domain was specified as air at 293.15 K and 1 atm. The boundary conditions were then specified. One cross section served as the inlet with velocity 1.0624 m/s and temperature 300K while the other served as the outlet with zero gauge pressure, no viscous stress and thermal insulation. The remaining surfaces were set as walls with wall function condition. The cylindrical wall was maintained at a constant temperature of 400 K and the spheres were maintained at a constant temperature of 300 K. Extremely coarse meshing (18435 elements) was used and the model was simulated using COMSOL (4.2a) to obtain the results.

## 4. Results and Discussion

### 4.1 N=4 model

The following results were obtained when N=4 packed bed 3D model was simulated using COMSOL Multiphysics (4.2a)

#### 4.1.1 Velocity Field

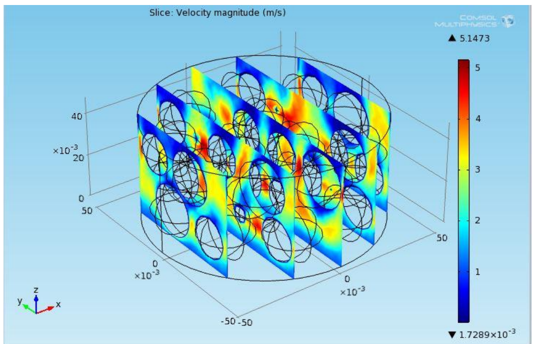


**Figure 3:** Velocity Plot (Surface) N=4

As shown in Figure 3, velocity increases as area decreases. This is in agreement with the continuity equation. The maximum velocity in the flow field is 5.1473 m/s. In the line plot, as shown in Figure 4, the velocity is zero wherever there is a packing (line is passing through the packing). Line passes through the coordinates (-5.08, 0, 3.4); (0, 0, 3.4).

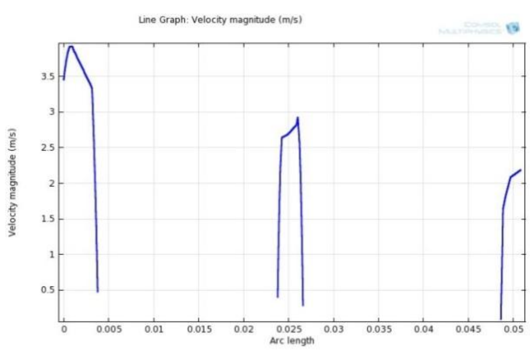


**Figure 4:** Velocity Plot (Line) N=4

Area plot is shown in Figure 5. The surface coordinates for the area are (-5.08, 0, 2.3); (0, -5.08, 2.3); (5.08, 0, 2.3). The maximum velocity in this cut surface is 3.9363 m/s.

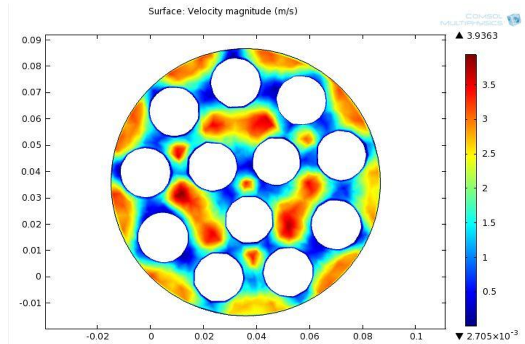


**Figure 5:** Velocity Plot (Area) N=4

#### 4.1.2 Pressure Field

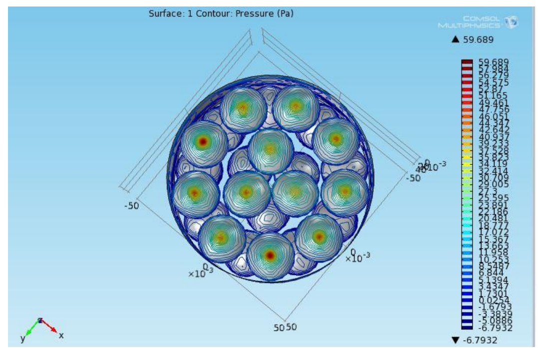


**Figure 6:** Pressure Contour N=4

It can be seen that there is a pressure drop across the length of the packed bed and this can be attributed to the fact that there is a net increase in the velocity along the packed bed. As shown in Figure 6, pressure is maximum at the stagnation point (velocity=0), in accordance with the momentum equation. The maximum pressure is 59.689 Pa. The same thing applies for the pressure dip at contractions where velocity magnitudes are high. Due to high velocities at contractions, turbulent boundary layer grows rapidly and due to adverse pressure gradient, flow separation occurs. This results in wake formation behind the separation points.

### 4.1.3 Temperature Profile

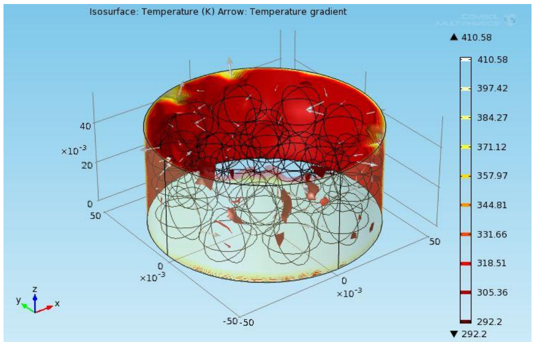


**Figure 7:** Temperature Gradient (Arrow Plot) N=4

As shown in Figure 7, the temperature is maximum at the cylindrical wall in accordance with the boundary condition. From the continuity equation, velocity increases when area decreases and hence the convective heat flux increases which further creates a temperature gradient.

### 4.2 N=8 model

The following results were obtained when N=8 packed bed 3D model was simulated using COMSOL Multiphysics (4.2a)

### 4.2.1 Velocity Field

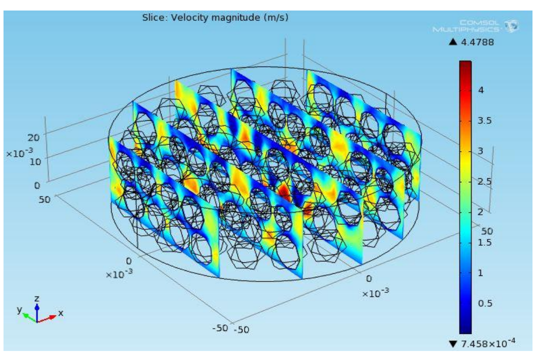


**Figure 8:** Velocity Plot (Surface) N=8

As shown in Figure 8, velocity increases as area decreases. This is in agreement with the continuity equation. The maximum velocity is 4.4788 m/s. The maximum velocity here is slightly less than the one obtained for the N=4 model. This can be attributed to the fact that there is more obstruction to flow in this geometry.

### 4.2.2 Pressure Field

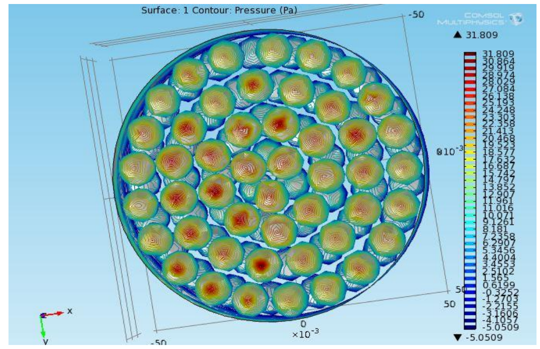


**Figure 8:** Pressure Contour N=8

As shown in Figure 8, the nature of the pressure contours is similar to the one we obtained for the N=4 model. Here the maximum pressure is 31.809 Pa.

### 4.2.3 Temperature Profile

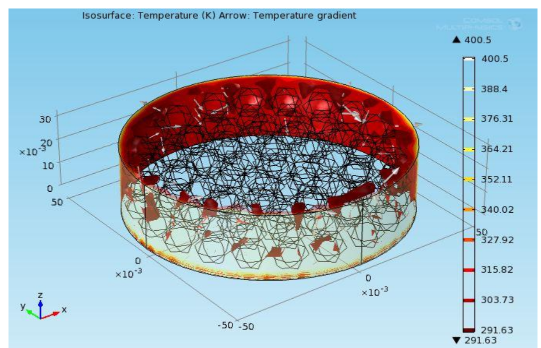


**Figure 9:** Temperature Gradient (Arrow Plot) N=8

As shown in Figure 9, the nature of the temperature profile obtained for this model is similar to the one obtained for the N=4 model. Here the maximum temperature is 400.5 K

## 5. Conclusion

An approach to fluid flow in low tube-to-particle diameter fixed beds is needed that is general enough to be applicable for reactor design purposes, but that retains the detailed flow features that contribute to transport of heat and mass and to strong local gradients that could influence reaction kinetics. This approach should provide a link to bed structure, so that, if packing or packing characteristics are known, flow features, transport rates, and reactor performance can be rapidly assessed. Computational fluid dynamics simulations of flow through packed-bed structures can provide highly detailed and reliable information about the temperature and flow fields. In this study, the flow of air through packed beds with spherical packing for N=4, and N=8 geometries for three dimensional models were analyzed. Plots for velocity field, pressure contours and temperature profiles across the sub domains were obtained. Further, the results obtained through CFD (COMSOL Multi-physics 4.2a) were analyzed and validated with the literature data. The nature of the results for the N=4 and N=8 models were similar but there was a difference in the values of the velocity, pressure and temperature. The values of the results obtained for the N=8 model can be considered as more practical since the packing arrangement is closer to reality.

It is possible to develop models for even higher N values which are closer to reality but their modeling is difficult because of complicated geometry and presence of wall effects across the entire radius of the bed. The challenge for the future is to use the information that will be available to gain knowledge and understanding which will be used to develop reduced models that are detailed enough for design purposes, but still intuitively understandable and computationally tractable. Some of the recent tools of information technology will be of use in this endeavor.

## 6. Nomenclature

N = Tube to particle diameter ratio, $\beta$ = void fraction, $u_o$ = superficial velocity, $d_p$ = particle diameter, k = thermal conductivity, k = turbulent kinetic energy, $\mu_T$ = turbulent viscosity, $\varepsilon$ = rate of dissipation of kinetic energy

## 7. References


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